

hyocholic acid

Inchi:	InChI=1S/C24H40O5/c1-13(4-7-19(26)27)15-5-6-16-20-17(9-11-23(15,16)2)24(3)10-8-14
InchiKey:	DKPMWHFRUGMUKF-UHFFFAOYSA-N
Formula:	C24H40O5
SMILES:	CC(CCC(=O)O)C1CCC2C3C(O)C(O)C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	408.58

Physical Properties

Property code	Value	Unit	Source
gf	-402.18	kJ/mol	Joback Method
hf	-1096.63	kJ/mol	Joback Method
hfus	48.21	kJ/mol	Joback Method
hvap	138.45	kJ/mol	Joback Method
log10ws	-4.35		Aqueous Solubility Prediction Method
logp	3.449		Crippen Method
mcvol	330.630	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
tb	1191.44	K	Joback Method
tc	1486.83	K	Joback Method
tf	714.97	K	Joback Method
vc	1.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.50	J/molxK	1191.44	Joback Method
cpg	1513.96	J/molxK	1240.67	Joback Method
cpg	1566.65	J/molxK	1289.90	Joback Method
cpg	1624.27	J/molxK	1339.13	Joback Method
cpg	1687.52	J/molxK	1388.36	Joback Method
cpg	1757.10	J/molxK	1437.60	Joback Method
cpg	1833.71	J/molxK	1486.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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